Limit theorems for the interference terms of discrete-time quantum walks on the line

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The probability distributions of discrete-time quantum walks have been often investigated, and many interesting properties of them have been discovered. The probability that the walker can be find at a position is defined by diagonal elements of the density matrix. On the other hand, although non-diagonal elements of the density matrices have an important role to quantify quantumness, they have not received attention in quantum walks. We focus on the non-diagonal elements of the density matrices for discrete-time quantum walks on the line and derive limit theorems for them.

Keywords: 2-state quantum walk, density matrix, interference term

1 Introduction

The discrete-time quantum walk (QW) is considered as a quantum analogous of the random walk which expresses the random motion of particles, and many interesting properties of the QWs have been discovered [1, 2, 3, 4]. Although QWs have simple dynamics in analogy with random walks, the behavior of quantum walkers is different from that of random walkers. The properties of the QWs are available to quantum information theory in which we can expect QWs to give a sizable contribution to quantum computer. Indeed, compared with classical search algorithms, the corresponding quantum algorithms based on QWs produce exponential speed-up. The difference between QWs and random walks is seen in probability distributions. The probability that the quantum walker on the line is found at position $x \in \mathbb{Z} = \{0, \pm 1, \pm 2, \ldots\}$ is defined by sum of diagonal elements in the density matrix at position x. The probability distributions of the QWs have been analyzed mainly and many limit theorems for them have been proved. Meanwhile, non-diagonal elements of the density matrices have got little attention in quantum walks and the behavior of them have not clarified. So, the aim of our paper is to get the characteristics of the non-diagonal elements in QWs. Non-diagonal elements of the density matrix, which are often called interference terms, show the distinction between quantum and classical states. If the particle takes mixed state, non-diagonal elements of the density matrix are necessarily null. That is, the interference terms of the density matrix for classical state are vanished. When the state of particles is not classical, they can become non-zero values. The non-diagonal elements of the density matrix have an important role when we characterize quantumness of particles. In quantum mechanics they are the essential values to express decoherence, which has been also investigated in QWs, both numerically and analytically [3, 5, 6, 7, 8].

The direct study for non-diagonal elements of the density matrices in QWs has not been done. Instead, we have analyzed the von Neumann entropy to quantify the entanglement, which is defined by density matrices [9, 10, 11, 12, 13]. Carneiro et al. [11] numerically

computed the von Neumann entropy of QWs. In Abal et al. [9] and Annabestani et al. [10], analytical results were obtained. Liu and Petulante [13] and Ide et al. [12] derived limit theorems for the von Neumann entropy.

The present paper is organized as follows. In Sect. 2, we introduce the notations of 2-state QWs on the line and give the time evolution rule and probability distribution of the QWs. In Sect. 3, we present two limit theorems for interference terms of density matrices as our main result. Section 4 is devoted to proofs of the limit theorems. Summary is mentioned in the last section. In appendix A, we show limit theorems for 3-state Grover walks on the line.

2 Definition of the 2-state QW on the line

In this section we define the 2-state QW on the line. Let $|x\rangle$ ($x \in \mathbb{Z} = \{0, \pm 1, \pm 2, \ldots\}$) be infinite components vectors which denote the position of the walker. Here, x-th component of $|x\rangle$ is 1 and the other is 0. Let $|\psi_t(x)\rangle \in \mathbb{C}^2$ be the amplitude of the walker at position x at time $t \in \{0, 1, 2, \ldots\}$, where $\mathbb{C}$ is the set of complex numbers. The walk at time t is expressed by

$$|\Psi_t\rangle = \sum_{x\in\mathbb{Z}} |x\rangle \otimes |\psi_t(x)\rangle \,. \tag{1}$$

The time evolution of the walk is described by the following unitary matrix:

$$U = \begin{bmatrix} u_{00} & u_{01} \\ u_{10} & u_{11} \end{bmatrix}, \tag{2}$$

where $u_{j_1 j_2} \in \mathbb{C}\,(j_1, j_2 \in \{0, 1\})$. In the present paper, we take the components of U as $u_{00} = -u_{11} = \cos\theta, u_{01} = u_{10} = \sin\theta$ or $u_{00} = u_{11} = \cos\theta, -u_{01} = u_{10} = \sin\theta$ with $\theta \in (0, 2\pi)\,(\theta \neq \pi/2, \pi, 3\pi/2)$. Then the evolution is determined by

$$|\psi_{t+1}(x)\rangle = P\,|\psi_t(x+1)\rangle + Q\,|\psi_t(x-1)\rangle\,, \tag{3}$$

where $P = |0\rangle\langle 0| U, Q = |1\rangle\langle 1| U$ and

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix},\ |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{4}$$

The probability that the quantum walker X_t is at position x at time t, $\mathbb{P}(X_t = x)$, is defined by

$$\mathbb{P}(X_t = x) = \sum_{j=0}^{1} \langle j|\,\rho_t(x)\,|j\rangle\,, \tag{5}$$

where $\rho_t(x) = |\psi_t(x)\rangle\langle\psi_t(x)|$ are the density matrices at position x at time t.

3 Main results

We will show two limit theorems for the non-diagonal elements of the density matrices $\rho_t(x)$. A limit theorem for the diagonal elements $\langle j|\,\rho_t(x)\,|j\rangle$ ($j \in \{0, 1\}$), that is probability distribution, has been given already by Konno [14, 15] and Grimmett et al. [16]. Konno [14, 15] obtained the limit theorem for the probability distribution of X_t/t as $t \to \infty$ by using path counting method. Grimmett et al. [16] also computed it by the Fourier analysis. From

their results, for the 2-state QWs starting from the origin with $|\psi_0(0)\rangle = \alpha|0\rangle + \beta|1\rangle$ and $|\alpha|^2 + |\beta|^2 = 1$, we see the following limit theorem.
For $u_{00}u_{01}u_{10}u_{11} \neq 0$ and $r = 0, 1, 2, \ldots$, we have

$$\lim_{t\to\infty} \sum_{x\in\mathbb{Z}} \left(\frac{x}{t}\right)^r \sum_{j=0}^{1} \langle j|\,\rho_t(x)\,|j\rangle = \lim_{t\to\infty} \mathbb{E}\left[\left(\frac{X_t}{t}\right)^r\right] = \int_{-\infty}^{\infty} y^r g(y)\,dy, \tag{6}$$

where

$$\begin{aligned} g(x) =& \frac{\sqrt{1-|u_{00}|^2}}{\pi(1-x^2)\sqrt{|u_{00}|^2 - x^2}} I_{(-|u_{00}|,|u_{00}|)}(x) \\ & \times \left\{1 - \left(|\alpha|^2 - |\beta|^2 + \frac{\alpha u_{00}\overline{\beta u_{01}} + \overline{\alpha u_{00}}\beta u_{01}}{|u_{00}|^2}\right) x\right\}, \end{aligned} \tag{7}$$

$I_A(x) = 1$ if $x \in A$, $I_A(x) = 0$ if $x \notin A$ and $\mathbb{E}(Y)$ means the expected value of Y. We compare the limit function $g(x)$ with probability distribution of the 2-state QW at time $t = 1000$ in Fig. 1.

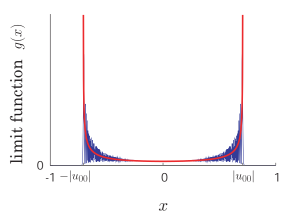


Fig. 1. The limit function $g(x)$ (thick line) and probability distribution of X_t/t at time $t = 1000$ (thin line) with $u_{00} = u_{01} = u_{10} = -u_{11} = 1/\sqrt{2}, \alpha = 1/\sqrt{2}, \beta = -i/\sqrt{2}$

In the present paper, we focus on the non-diagonal elements $\langle 0|\,\rho_t(x)\,|1\rangle$ in the density matrices $\rho_t(x)$, which are often called the interference terms in quantum mechanics, and derive limit theorems for them. At first, when we consider the 2-state quantum walks starting with any initial state, we can obtain the following relation between the interference terms and the moments of X_t/t.

Theorem 1 *For $r = 0, 1, 2, \ldots$, we have*

$$\lim_{t\to\infty} \sum_{x\in\mathbb{Z}} \left(\frac{x}{t}\right)^r \Re(\langle 0|\,\rho_t(x)\,|1\rangle) = (\det U)\frac{s}{2c} \lim_{t\to\infty} \mathbb{E}\left[\left(\frac{X_t}{t}\right)^{r+1}\right], \tag{8}$$

where $c = \cos\theta, s = \sin\theta$ and $\Re(z)$ denotes the real part of $z \in \mathbb{C}$.

Moreover, if we assume that the 2-state quantum walks starting from the origin with $|\psi_0(0)\rangle = \alpha|0\rangle + \beta|1\rangle$ and $|\alpha|^2 + |\beta|^2 = 1$, the limit theorem is given as follows.

Theorem 2 *For $r = 0, 1, 2, \ldots$, we see*

$$\lim_{t\to\infty} \sum_{x\in\mathbb{Z}} \left(\frac{x}{t}\right)^r \langle 0|\,\rho_t(x)\,|1\rangle = \int_{-\infty}^{\infty} y^r \left\{f^{(R)}(y) + i f^{(I)}(y)\right\} dy, \tag{9}$$

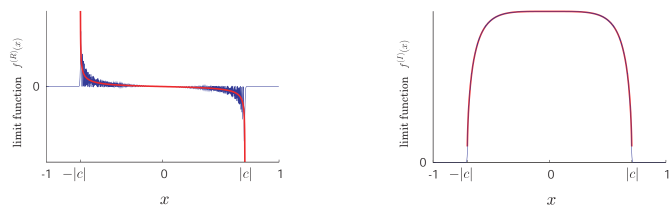
where

$$f^{(R)}(x) = (\det U)\,\frac{s}{2c}x\cdot\frac{|s|}{\pi(1-x^2)\sqrt{c^2-x^2}} \times\left[1-\left\{|\alpha|^2-|\beta|^2-(\det U)\frac{s}{c}(\alpha\overline{\beta}+\overline{\alpha}\beta)\right\}x\right]I_{(-|c|,|c|)}(x), \tag{10}$$

$$f^{(I)}(x) = \frac{|s|\Im(\alpha\overline{\beta})}{\pi c^2}\cdot\frac{\sqrt{c^2-x^2}}{1-x^2}I_{(-|c|,|c|)}(x), \tag{11}$$

and $\Im(z)$ *is the imaginary part of* $z\in\mathbb{C}$.

Figure 2 shows a comparison of the limit functions $f^{(R)}(x)$, $f^{(I)}(x)$ and non-diagonal elements of the density matrices $\rho_t(x)$.



(a) $f^{(R)}(x), \Re(\langle 0|\rho_t(x)|1\rangle)$ (b) $f^{(I)}(x), \Im(\langle 0|\rho_t(x)|1\rangle)$

Fig. 2. The limit function $f^{(R)}(x), f^{(I)}(x)$ (thick line) and $\Re(\langle 0|\rho_t(x)|1\rangle), \Im(\langle 0|\rho_t(x)|1\rangle)$ at time $t=1000$ (thin line) with $u_{00}=-u_{11}=c=1/\sqrt{2}, u_{01}=u_{10}=s=1/\sqrt{2}, \alpha=1/\sqrt{2}, \beta=-i/\sqrt{2}$

4 Proof of Theorems

4.1 Proof of Theorem 1

Our proof is based on the Fourier analysis introduced by Grimmett et al. [16]. The Fourier transform $|\hat{\Psi}_t(k)\rangle$ ($k\in[-\pi,\pi)$) of $|\psi_t(x)\rangle$ is given by

$$|\hat{\Psi}_t(k)\rangle = \sum_{x\in\mathbb{Z}} e^{-ikx}\,|\psi_t(x)\rangle\,. \tag{12}$$

By the inverse Fourier transform, we have

$$|\psi_t(x)\rangle = \int_{-\pi}^{\pi} e^{ikx}\,|\hat{\Psi}_t(k)\rangle\,\frac{dk}{2\pi}. \tag{13}$$

From Eqs. (3) and (12), the time evolution of $|\hat{\Psi}_t(k)\rangle$ becomes

$$|\hat{\Psi}_{t+1}(k)\rangle = \hat{U}(k)\,|\hat{\Psi}_t(k)\rangle\,, \tag{14}$$

where $\hat{U}(k)=R(k)U$ and $R(k)=e^{ik}|0\rangle\langle 0|+e^{-ik}|1\rangle\langle 1|$. Equation (14) implies

$$|\hat{\Psi}_t(k)\rangle = \hat{U}(k)^t\,|\hat{\Psi}_0(k)\rangle\,. \tag{15}$$

The eigenvalues $\lambda_j(k)\,(j\in\{1,2\})$ of the unitary matrix $\hat{U}(k)$ are

$$\lambda_j(k)=\begin{cases} ic\sin k-(-1)^j\sqrt{1-c^2\sin^2 k} & (u_{00}=-u_{11}=c,u_{01}=u_{10}=s),\\ c\cos k-i(-1)^j\sqrt{1-c^2\cos^2 k} & (u_{00}=u_{11}=c,-u_{01}=u_{10}=s),\end{cases} \tag{16}$$

and the eigenvectors corresponding to $\lambda_j(k)$ take the following form

$$\begin{cases} \begin{bmatrix} se^{ik}\\ -c\cos k-(-1)^j\sqrt{1-c^2\sin^2 k}\end{bmatrix} & (u_{00}=-u_{11}=c,u_{01}=u_{10}=s),\\ \begin{bmatrix} se^{ik}\\ i\left\{c\sin k+(-1)^j\sqrt{1-c^2\cos^2 k}\right\}\end{bmatrix} & (u_{00}=u_{11}=c,-u_{01}=u_{10}=s).\end{cases} \tag{17}$$

By the eigenvalues $\lambda_j(k)$ and the normalized eigenvectors $|v_j(k)\rangle$, Eq. (15) can be rewritten as

$$|\hat{\Psi}_t(k)\rangle=\hat{U}(k)^t\sum_{j=1}^{2}\langle v_j(k)|\hat{\Psi}_0(k)\rangle\,|v_j(k)\rangle=\sum_{j=1}^{2}\lambda_j(k)^t\,\langle v_j(k)|\hat{\Psi}_0(k)\rangle\,|v_j(k)\rangle\,. \tag{18}$$

From now, we will prove Theorem 1. At first, in order to express the left-side hand of Eq. (8) by the Fourier transform, we compute as follows:

$$\begin{aligned}
&\sum_{x\in\mathbb{Z}}x^r\Re(\langle 0|\,\rho_t(x)\,|1\rangle)=\frac{1}{2}\sum_{x\in\mathbb{Z}}x^r\left\{\langle 0|\,\rho_t(x)\,|1\rangle+\langle 1|\,\rho_t(x)\,|0\rangle\right\}\\
=&\frac{1}{2}\int_{-\pi}^{\pi}\langle\hat{\Psi}_t(k)|\,J^+\left(D^r\,|\hat{\Psi}_t(k)\rangle\right)\frac{dk}{2\pi}\\
=&\frac{(t)_r}{2}\int_{-\pi}^{\pi}\left\{\sum_{j=1}^{2}h_j(k)^r|\,\langle v_j(k)|\hat{\Psi}_0(k)\rangle\,|^2\,\langle v_j(k)|J^+|v_j(k)\rangle\right.\\
&+(\overline{\lambda_1(k)}\lambda_2(k))^t h_2(k)^r\,\langle v_2(k)|\hat{\Psi}_0(k)\rangle\,\langle v_1(k)|J^+|v_2(k)\rangle\,\overline{\langle v_1(k)|\hat{\Psi}_0(k)\rangle}\\
&\left.+(\lambda_1(k)\overline{\lambda_2(k)})^t h_1(k)^r\,\langle v_1(k)|\hat{\Psi}_0(k)\rangle\,\langle v_2(k)|J^+|v_1(k)\rangle\,\overline{\langle v_2(k)|\hat{\Psi}_0(k)\rangle}\right\}\frac{dk}{2\pi}\\
&+O(t^{r-1}),
\end{aligned} \tag{19}$$

where $J^+=|0\rangle\langle 1|+|1\rangle\langle 0|$, $h_j(k)=D\lambda_j(k)/\lambda_j(k)\,(j\in\{1,2\})$, $D=i(d/dk)$ and $(t)_r=t(t-1)\times\cdots\times(t-r+1)$. By using the Riemann-Lebesgue lemma, we have

$$\lim_{t\to\infty}\sum_{x\in\mathbb{Z}}\left(\frac{x}{t}\right)^r\Re(\langle 0|\,\rho_t(x)\,|1\rangle)=\frac{1}{2}\int_{-\pi}^{\pi}\left\{\sum_{j=1}^{2}h_j(k)^r|\,\langle v_j(k)|\hat{\Psi}_0(k)\rangle\,|^2\,\langle v_j(k)|J^+|v_j(k)\rangle\right\}\frac{dk}{2\pi}. \tag{20}$$

Since we easily find $\langle v_j(k)|J^+|v_j(k)\rangle=(\det\,U)\frac{s}{c}h_j(k)$,

$$\begin{aligned}
\lim_{t\to\infty}\sum_{x\in\mathbb{Z}}\left(\frac{x}{t}\right)^r\Re(\langle 0|\,\rho_t(x)\,|1\rangle)=&(\det\,U)\frac{s}{2c}\int_{-\pi}^{\pi}\left\{\sum_{j=1}^{2}h_j(k)^{r+1}|\,\langle v_j(k)|\hat{\Psi}_0(k)\rangle\,|^2\right\}\frac{dk}{2\pi}\\
=&(\det\,U)\frac{s}{2c}\lim_{t\to\infty}\mathbb{E}\left[\left(\frac{X_t}{t}\right)^{r+1}\right].
\end{aligned} \tag{21}$$

□

4.2 Proof of Theorem 2

The real part $f^{(R)}(x)$ can be obtained from Theorem 1 and the result in Konno [14, 15] as follows:

$$\begin{aligned}\lim_{t\to\infty}\sum_{x\in\mathbb{Z}}\left(\frac{x}{t}\right)^r \Re(\langle 0|\,\rho_t(x)\,|1\rangle) =& (\det U)\frac{s}{2c}\int_{-\infty}^{\infty} y^{r+1}\,\frac{|s|}{\pi(1-y^2)\sqrt{c^2-y^2}} \\ &\times\left[1-\left\{|\alpha|^2-|\beta|^2-(\det U)\frac{s}{c}(\alpha\overline{\beta}+\overline{\alpha}\beta)\right\}y\right] I_{(-|c|,|c|)}(y)\,dy \\ =& \int_{-\infty}^{\infty} y^r\,(\det U)\,\frac{s}{2c}y\cdot\frac{|s|}{\pi(1-y^2)\sqrt{c^2-y^2}} \\ &\times\left[1-\left\{|\alpha|^2-|\beta|^2-(\det U)\frac{s}{c}(\alpha\overline{\beta}+\overline{\alpha}\beta)\right\}y\right] I_{(-|c|,|c|)}(y)\,dy.\end{aligned} \tag{22}$$

Next, we calculate the imaginary part $f^{(I)}(x)$. In a similar fashion as the proof of Theorem 1,

$$\lim_{t\to\infty}\sum_{x\in\mathbb{Z}}\left(\frac{x}{t}\right)^r \Im(\langle 0|\,\rho_t(x)\,|1\rangle) = \frac{1}{2i}\int_{-\pi}^{\pi}\left\{\sum_{j=1}^{2} h_j(k)^r|\,\langle v_j(k)|\psi_0(0)\rangle\,|^2\,\langle v_j(k)|J^-|v_j(k)\rangle\right\}\frac{dk}{2\pi}, \tag{23}$$

where $\Im(z)$ denotes the imaginary part of $z\in\mathbb{C}$ and $J^-=|1\rangle\langle 0|-|0\rangle\langle 1|$. Note that the initial state becomes $|\hat{\Psi}_0(k)\rangle=|\psi_0(0)\rangle=\alpha\,|0\rangle+\beta\,|1\rangle$. After putting $h_j(k)=y\,(j\in\{1,2\})$, we get

$$\lim_{t\to\infty}\sum_{x\in\mathbb{Z}}\left(\frac{x}{t}\right)^r \Im(\langle 0|\,\rho_t(x)\,|1\rangle) = \int_{-\infty}^{\infty} y^r\,\frac{|s|\Im(\alpha\overline{\beta})}{\pi c^2}\cdot\frac{\sqrt{c^2-y^2}}{1-y^2}I_{(-|c|,|c|)}(y)\,dy. \tag{24}$$

Combining Eqs. (22) and (24), we complete the proof of Theorem 2.

□

5 Summary

In this section, we mention discussion and conclusion for our results. In the present paper, we investigated non-diagonal elements in the density matrices of discrete-time 2-state QWs on the line. Non-diagonal elements of the density matrix are called interference terms and they are important values to quantify decoherence of quantum particles. In Sect. 3 we gave two limit theorems for the interference terms of density matrices at position $x\in\mathbb{Z}$ in 2-state QWs. One is the limit theorem for the QW starting with any initial state, the other is the limit theorem when the walker starts from the origin. Theorem 1 showed the relation between the interference terms of the QW starting with any initial state and the r-th moments $(r=0,1,2,\ldots)$ of X_t/t. From Theorem 2, if the walker starts from the origin, the limit function which denotes the imaginary part of the interference terms always becomes an even function regardless of the initial state at the origin. One of the interesting problems is to get the relations between decoherent process and QWs, that is, expression of transition from quantum state to classical state by QWs. Chisaki et al. [18] studied crossover from QW

to classical random walk. So, it would be interesting to discuss the relation between our results and their results. If we can construct the decoherent process by QWs, innovative investigations may start in quantum mechanics.

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Appendix A

In this appendix, we consider the 3-state Grover walk on the line and will show two limit theorems for the non-diagonal elements of the density matrices. The difference between the 2-state QWs defined in Sect. 2 and the 3-state Grover walk is whether localization occurs or not. The probability distribution of the 2-state QWs doesn't localized, while the 3-state Grover walk is known as one of the models in which localization can occur. The 3-state Grover walk on the line is defined as follows. The amplitudes of the walker at position $x \in \mathbb{Z}$ at time $t \in \{0,1,2,\ldots\}$ are given by $|\psi_t(x)\rangle \in \mathbb{C}^3$. The time evolution of the walk is determined by the Grover matrix $G = \frac{2}{3}\sum_{j_1=0}^{2}\sum_{j_2=0}^{2} |j_1\rangle\langle j_2| - \sum_{j=0}^{2} |j\rangle\langle j|$ with

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix},\ |1\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix},\ |2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{A.1}$$

The amplitudes $|\psi_t(x)\rangle$ evolve by the following rule:

$$|\psi_{t+1}(x)\rangle = P_0 |\psi_t(x+1)\rangle + P_1 |\psi_t(x)\rangle + P_2 |\psi_t(x-1)\rangle, \tag{A.2}$$

where $P_0 = |0\rangle\langle 0| G, P_1 = |1\rangle\langle 1| G, P_2 = |2\rangle\langle 2| G$. Inui et al. [17] focused on the probability distribution $\mathbb{P}(X_t = x) = \sum_{j=0}^{2} \langle j| \rho_t(x) |j\rangle$ and got a long-time limit theorem for $\sum_{x\in\mathbb{Z}} \left(\frac{x}{t}\right)^r \sum_{j=0}^{2} \langle j| \rho_t(x) |j\rangle = \mathbb{E}\left[(X_t/t)^r\right]$ (see Eq. (16) in [17]). Figure A.1 shows probability distribution of the 3-state Grover walk at time $t = 150$ with $|\psi_0(0)\rangle = 1/\sqrt{3}\,|0\rangle + i/\sqrt{3}\,|1\rangle + i/\sqrt{3}\,|2\rangle$.

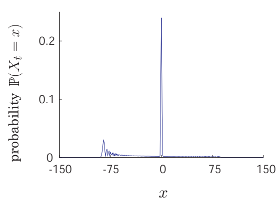


Fig. A.1. Probability distribution of the 3-state Grover walk at time $t = 150$ starting from the origin with the initial state $|\psi_0(0)\rangle = 1/\sqrt{3}\,|0\rangle + i/\sqrt{3}\,|1\rangle + i/\sqrt{3}\,|2\rangle$

On the other hand, we derive limit theorems for the interference terms $\langle j_1| \rho_t(x) |j_2\rangle$ ($(j_1, j_2) \in \{(0,1),(0,2),(1,2)\}$). The proofs of theorems are given as well as the ones of Theorems 1 and 2. So, we will omit them.

For the 3-state Grover walk starting with any initial state, we can obtain the relations between the interference terms and the moments of X_t/t.

Theorem A.1 *As $t \to \infty$, the summations of $(x/t)^r \Re(\langle j_1| \rho_t(x) |j_2\rangle)$ $(r = 0,1,2,\ldots)$ all over $x \in \mathbb{Z}$ are calculated as follows:*

1. *For $r = 0$, we have*

$$\lim_{t\to\infty} \sum_{x\in\mathbb{Z}} \Re(\langle j_1| \rho_t(x) |j_2\rangle) = \begin{cases} \Delta_{01}^{(R)} + \frac{1}{2}\lim_{t\to\infty} \mathbb{E}\left[\frac{X_t}{t}\right] - \frac{1}{2}\lim_{t\to\infty}\mathbb{E}\left[\left(\frac{X_t}{t}\right)^2\right] & (j_1 = 0, j_2 = 1), \\ \Delta_{02}^{(R)} + \frac{1}{4} - \frac{5}{4}\lim_{t\to\infty}\mathbb{E}\left[\left(\frac{X_t}{t}\right)^2\right] & (j_1 = 0, j_2 = 2), \\ \Delta_{12}^{(R)} - \frac{1}{2}\lim_{t\to\infty} \mathbb{E}\left[\frac{X_t}{t}\right] - \frac{1}{2}\lim_{t\to\infty}\mathbb{E}\left[\left(\frac{X_t}{t}\right)^2\right] & (j_1 = 1, j_2 = 2), \end{cases} \tag{A.3}$$

where

$$\Delta^{(R)}_{j_1j_2} = \begin{cases} \int_{-\pi}^{\pi} \frac{dk}{2\pi}\, \frac{1}{2} |\langle v(k)|\hat{\Psi}_0(k)\rangle|^2 \langle v(k)|J^+_{j_1j_2}|v(k)\rangle & ((j_1,j_2)=(0,1),(1,2)),\\ \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left\{ \frac{1}{2} |\langle v(k)|\hat{\Psi}_0(k)\rangle|^2 \langle v(k)|J^+_{j_1j_2}|v(k)\rangle \right. & \\ \qquad \left. -\frac{1}{4} |\langle v(k)|\hat{\Psi}_0(k)\rangle|^2 \right\} & ((j_1,j_2)=(0,2)), \end{cases} \tag{A.4}$$

and $|\hat{\Psi}_0(k)\rangle = \sum_{x\in\mathbb{Z}} e^{-ikx} |\psi_0(x)\rangle$ *and* $J^+_{j_1j_2} = |j_1\rangle\langle j_2| + |j_2\rangle\langle j_1|$. *The vector* $|v(k)\rangle$ *is the normalized eigenvector corresponding to the eigenvalue* $\lambda = 1$ *of the unitary matrix* $R(k)G$ *with* $R(k) = e^{ik}|0\rangle\langle 0| + |1\rangle\langle 1| + e^{-ik}|2\rangle\langle 2|$*:*

$$|v(k)\rangle = \sqrt{\frac{2}{5+\cos k}} \begin{bmatrix} 1 \\ (1+e^{-ik})/2 \\ e^{-ik} \end{bmatrix}. \tag{A.5}$$

2. *For* $r = 1, 2, \ldots$, *we have*

$$\lim_{t\to\infty} \sum_{x\in\mathbb{Z}} \left(\frac{x}{t}\right)^r \Re(\langle j_1|\,\rho_t(x)\,|j_2\rangle) \tag{A.6}$$

$$= \begin{cases} \frac{1}{2}\lim_{t\to\infty} \mathbb{E}\left[\left(\frac{X_t}{t}\right)^{r+1}\right] - \frac{1}{2}\lim_{t\to\infty} \mathbb{E}\left[\left(\frac{X_t}{t}\right)^{r+2}\right] & (j_1=0, j_2=1),\\ \frac{1}{4}\lim_{t\to\infty} \mathbb{E}\left[\left(\frac{X_t}{t}\right)^{r}\right] - \frac{5}{4}\lim_{t\to\infty} \mathbb{E}\left[\left(\frac{X_t}{t}\right)^{r+2}\right] & (j_1=0, j_2=2),\\ -\frac{1}{2}\lim_{t\to\infty} \mathbb{E}\left[\left(\frac{X_t}{t}\right)^{r+1}\right] - \frac{1}{2}\lim_{t\to\infty} \mathbb{E}\left[\left(\frac{X_t}{t}\right)^{r+2}\right] & (j_1=1, j_2=2). \end{cases} \tag{A.7}$$

Particularly, when the 3-state Grover walk starts from the origin with $|\psi_0(0)\rangle = \alpha|0\rangle + \beta|1\rangle + \gamma|2\rangle$ and $|\alpha|^2+|\beta|^2+|\gamma|^2 = 1$, we can get the specific limit theorem for the interference terms.

Theorem A.2 *For* $r = 0, 1, 2, \ldots$, *we see*

$$\lim_{t\to\infty} \sum_{x\in\mathbb{Z}} \left(\frac{x}{t}\right)^r \langle j_1|\,\rho_t(x)\,|j_2\rangle = \int_{-\infty}^{\infty} y^r \left\{ f^{(R)}_{j_1j_2}(y) + i f^{(I)}_{j_1j_2}(y) \right\} dy, \tag{A.8}$$

where

$$f^{(R)}_{j_1j_2}(x) = \begin{cases} \Delta^{(R)}_{01}\delta_0(x) + \frac{\sqrt{2}(c_0+c_1x+c_2x^2)}{4\pi\sqrt{1-3x^2}} \frac{x}{1+x} I_{(-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}})}(x) & (j_1=0,j_2=1),\\ \Delta^{(R)}_{02}\delta_0(x) + \frac{\sqrt{2}(c_0+c_1x+c_2x^2)}{4\pi\sqrt{1-3x^2}} \frac{1-5x^2}{2(1-x^2)} I_{(-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}})}(x) & (j_1=0,j_2=2),\\ \Delta^{(R)}_{12}\delta_0(x) - \frac{\sqrt{2}(c_0+c_1x+c_2x^2)}{4\pi\sqrt{1-3x^2}} \frac{x}{1-x} I_{(-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}})}(x) & (j_1=1,j_2=2), \end{cases} \tag{A.9}$$

$$f^{(I)}_{j_1j_2}(x) = \begin{cases} \Delta^{(I)}_{01}\delta_0(x) + \frac{(d_0+d_1x)\sqrt{1-3x^2}}{\pi} \frac{1}{\sqrt{2}(1+x)} I_{(-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}})}(x) & (j_1=0,j_2=1),\\ \Delta^{(I)}_{02}\delta_0(x) - \frac{(d_0+d_1x)\sqrt{1-3x^2}}{\pi} \frac{\sqrt{2}x}{1-x^2} I_{(-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}})}(x) & (j_1=0,j_2=2),\\ \Delta^{(I)}_{12}\delta_0(x) - \frac{(d_0+d_1x)\sqrt{1-3x^2}}{\pi} \frac{1}{\sqrt{2}(1-x)} I_{(-\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}})}(x) & (j_1=1,j_2=2), \end{cases} \tag{A.10}$$

and $\delta_0(x)$ denotes Dirac's δ-function at the origin. The coefficients are computed as follows:

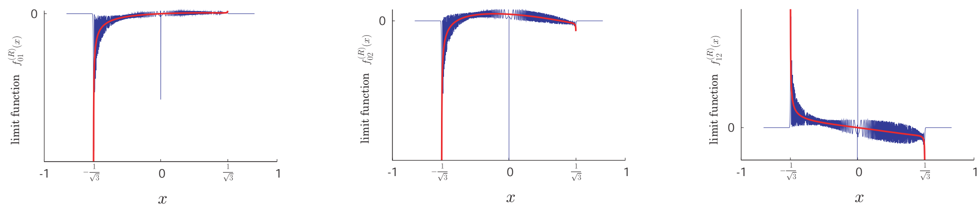
$$\Delta^{(R)}_{j_1j_2} = \begin{cases} \frac{\sqrt{6}}{36}\left(\left|\alpha+\frac{\beta}{2}\right|^2+\left|\gamma+\frac{\beta}{2}\right|^2\right) \\ +\left(1-\frac{29\sqrt{6}}{72}\right)\Re\left\{(2\alpha+\beta)(2\overline{\gamma}+\overline{\beta})\right\} \quad (j_1=0, j_2=1), \\ -\frac{\sqrt{6}}{72}\left(\left|\alpha+\frac{\beta}{2}\right|^2+\left|\gamma+\frac{\beta}{2}\right|^2\right) \\ +\left(2-\frac{115\sqrt{6}}{144}\right)\Re\left\{(2\alpha+\beta)(2\overline{\gamma}+\overline{\beta})\right\} \quad (j_1=0, j_2=2), \\ \frac{\sqrt{6}}{36}\left(\left|\alpha+\frac{\beta}{2}\right|^2+\left|\gamma+\frac{\beta}{2}\right|^2\right) \\ +\left(1-\frac{29\sqrt{6}}{72}\right)\Re\left\{(2\alpha+\beta)(2\overline{\gamma}+\overline{\beta})\right\} \quad (j_1=1, j_2=2), \end{cases} \tag{A.11}$$

$$\Delta^{(I)}_{j_1j_2} = \begin{cases} \left(2-\frac{5\sqrt{6}}{6}\right)\Im(\overline{\alpha}\beta+\overline{\beta}\gamma+2\gamma\overline{\alpha}) \quad (j_1=0, j_2=1), \\ \left(4-\frac{5\sqrt{6}}{3}\right)\Im(\overline{\alpha}\beta+\overline{\beta}\gamma+2\gamma\overline{\alpha}) \quad (j_1=0, j_2=2), \\ \left(2-\frac{5\sqrt{6}}{6}\right)\Im(\overline{\alpha}\beta+\overline{\beta}\gamma+2\gamma\overline{\alpha}) \quad (j_1=1, j_2=2), \end{cases} \tag{A.12}$$

and

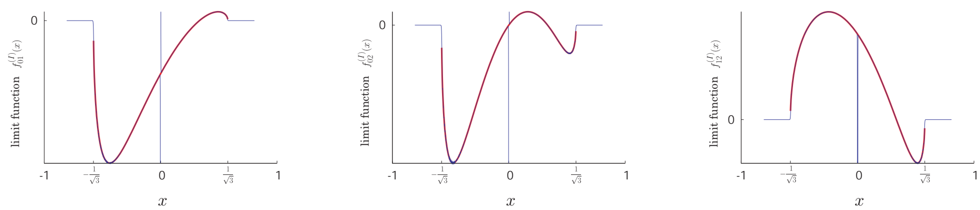
$$c_0 = |\alpha+\gamma|^2+2|\beta|^2, \tag{A.13}$$
$$c_1 = 2\left(-|\alpha-\beta|^2+|\gamma-\beta|^2\right), \tag{A.14}$$
$$c_2 = |\alpha-\gamma|^2-2\Re\left\{(2\alpha+\beta)(2\overline{\gamma}+\overline{\beta}))\right\}, \tag{A.15}$$
$$d_0 = \Im\left\{(\alpha+\gamma)\overline{\beta}\right\}, \tag{A.16}$$
$$d_1 = \Im\left\{\overline{\alpha}(\beta+\gamma)+(\overline{\alpha}+\overline{\beta})\gamma\right\}. \tag{A.17}$$

We should note $\Delta^{(R)}_{01}=\Delta^{(R)}_{12}, \Delta^{(I)}_{01}=\Delta^{(I)}_{12}$. When Theorems A.1 and A.2 are proved, we consider $J^+_{j_1j_2}=|j_1\rangle\langle j_2|+|j_2\rangle\langle j_1|$ (resp. $J^-_{j_1j_2}=|j_2\rangle\langle j_1|-|j_1\rangle\langle j_2|$) instead of $J^+=|0\rangle\langle 1|+|1\rangle\langle 0|$ (resp. $J^-=|1\rangle\langle 0|-|0\rangle\langle 1|$) in the proofs of Theorems 1 and 2. Examples of Theorem A.2 are presented in Figs. A.2 and A.3.



(a) $(j_1, j_2) = (0, 1)$ (b) $(j_1, j_2) = (0, 2)$ (c) $(j_1, j_2) = (1, 2)$

Fig. A.2. The limit function $f^{(R)}_{j_1 j_2}(x)$ (thick line) and $\Re(\langle j_1|\, \rho_t(x)\, |j_2\rangle)$ at time $t = 1000$ (thin line) with $\alpha = 1/\sqrt{3}$, $\beta = \gamma = i/\sqrt{3}$



(a) $(j_1, j_2) = (0, 1)$ (b) $(j_1, j_2) = (0, 2)$ (c) $(j_1, j_2) = (1, 2)$

Fig. A.3. The limit function $f^{(I)}_{j_1 j_2}(x)$ (thick line) and $\Im(\langle j_1|\, \rho_t(x)\, |j_2\rangle)$ at time $t = 1000$ (thin line) with $\alpha = 1/\sqrt{3}$, $\beta = \gamma = i/\sqrt{3}$